The effect of Temperature on Intermolecular Interaction of Monoethanolamine Absorption Process for CO2 Removal

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ABSTRACT
The reversible chemical absorption with an aqueous amine solution is mature and established technology for CO2 capture. The main objective of this study is to investigate the effect of temperature on intermolecular interaction of primary amine and CO2 in absorption process using Molecular Dynamic (MD) simulation. The simulation was run under condition NVE (200 ps) and NPT (1 ns) ensemble in Materials Studio 7.0 software. Three different temperature are used; 298K, 313K and 318K. The radial distribution function (RDF) is used to analyze the intermolecular interaction in the system. In binary (MEA+H2O) and tertiary (MEA+H2O+CO2) system, stronger interaction is observed at 318K compared to 298K and 313K. For binary system, the RDF for the (*g(r)*)value of hydrogen bonding is (1.75, 0.96), (1.75, 0.82) and (1.75, 0.81) at temperature 318K, 298K and 313K, respectively. The OMEA-HH2Ohydrogen bond has the highest peak of intermolecularinteraction based on RDF plot. The RDF value of hydrogen bonding for tertiary system is (1.75, 2.29), (1.75, 2.04) and (1.75, 1.56) at temperature 318K, 298K and 313K, respectively. The hydrogen bond of MEA+H2O has higher intermolecular interaction compared to Van der Waals bond of MEA+CO2. Due to weak intermolecular interaction between MEA and CO2, physical absorption is not preferable technology used for CO2 removal at low concentration of CO2. Therefore, reactive absorption process which involved reactions between MEA and CO2is more preferable technology used to increase CO2 removal efficiency.

KEYWORDS: Molecular Dynamic; Amine Absorption Process; Monoethanolamine; Carbon Dioxide Removal;Radial Distribution Function; Mean Square Displacement